

Aspirin

50-78-2 | DTXSID5020108

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 125 °C

Global applicability domain: Inside

Local applicability domain index: 9.29e-01

Confidence level: 4.97e-01

Nearest Neighbors from the Training Set

Image not found

Aspirin

Measured: 135

Predicted: 125

Image not found

Monomethyl phthalate

Measured: 83.0

Predicted: 116

Image not found

Benzoic acid, 4-(acetyloxy)-

Measured: 193

Predicted: 140

Image not found

Monobutyl phthalate

Measured: 73.5

Predicted: 96.8